

## 08-Inorganic and Mineralogical Crystallography

257

type the increase of Mo and V<sup>4+</sup> content gives rise to the uniformity of Me-O bonds. Connections between octahedron layers tend to release. Disordering becomes most pronounced when the compound possesses a VMo<sub>3</sub>O<sub>11</sub> composition. The peculiarities of the VMo<sub>3</sub>O<sub>11</sub> structure are assumed to provide its best catalytic properties among V-Mo oxide compounds in acrolein oxidation to acrylic acid.

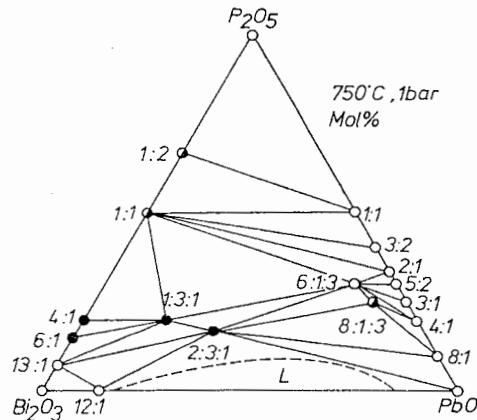
\*Alternative cell:  $a = 9.814\text{\AA}$ ,  $b = 11.440\text{\AA}$ ,  $c = 6.550\text{\AA}$ ,  $\beta = 94.27^\circ$

layer structures containing [Bi<sub>2</sub>O<sub>2</sub>] layers. Structure determinations are in preparation. Corresponding phosphates, arsenates and vanadates form solid solutions.

The authors thank the ICDD for financial support.

**PS-08.01.37 NEW COMPOUNDS IN THE SYSTEMS Bi<sub>2</sub>O<sub>3</sub>-PbO/Bi<sub>2</sub>O<sub>5</sub>/As<sub>2</sub>O<sub>5</sub>/V<sub>2</sub>O<sub>5</sub>.** By Y.C. Jie and W. Eysel, Mineralogisch-Petrographisches Institut, Universität Heidelberg, Germany

The system Bi<sub>2</sub>O<sub>3</sub>-PbO-P<sub>2</sub>O<sub>5</sub> was investigated between 600°C and 1000°C in air. The new phosphates PbBi<sub>3</sub>PO<sub>8</sub>, PbBi<sub>6</sub>P<sub>2</sub>O<sub>15</sub> and Bi<sub>12</sub>P<sub>2</sub>O<sub>23</sub> (full dots in the figure) were characterized by X-ray diffraction. For some other compounds (half



dots) high precision ion powder data were determined. For the new phosphates isostructural arsenates and vanadates as well as Sr compounds were synthesized (Table 1). According to the lattice parameters the various tetragonal, orthorhombic and monoclinic structures are closely related. The (pseudo-)tetragonal lattice parameter  $a \approx 11.7 = 3 \times 3.9 \text{ \AA}$  indicates

Table 1 STRUCTURAL DATA OF NEW COMPOUNDS.

T = tetragonal, O = orthorhombic,  
M = monoclinic

Compounds	Sym.	a(Å)	b(Å)	c(Å)	$\beta$ (°)
PbBi <sub>3</sub> PO <sub>8</sub>	T, I	11.756		15.604	
PbBi <sub>3</sub> AsO <sub>8</sub>		11.816		16.054	
PbBi <sub>3</sub> VO <sub>8</sub>		11.838		16.066	
SrBi <sub>3</sub> PO <sub>8</sub>	T, I	11.620		16.973	
SrBi <sub>3</sub> AsO <sub>8</sub>		11.769		16.439	
SrBi <sub>3</sub> VO <sub>8</sub>	O, I	11.981	11.678	16.266	
PbBi <sub>6</sub> P <sub>2</sub> O <sub>15</sub>	O, P	11.764	10.845	17.015	
PbBi <sub>6</sub> As <sub>2</sub> O <sub>15</sub>		11.943	11.007	17.267	
PbBi <sub>6</sub> V <sub>2</sub> O <sub>15</sub>		11.970	11.023	17.324	
Bi <sub>12</sub> P <sub>2</sub> O <sub>23</sub> *	M, P	12.210	11.440	15.767	92.28
Bi <sub>12</sub> As <sub>2</sub> O <sub>23</sub>		12.208	11.551	16.104	91.45
Bi <sub>12</sub> V <sub>2</sub> O <sub>23</sub>		12.193	11.579	16.163	91.13

**PS-08.01.38**

THE RESULTS OF MASS EMPLOYMENT OF THE UNIFICATION SYSTEM FOR THE QUANTITATIVE PHASE ANALYSIS PERFORMANCE BY X-RAY DIFFRACTION (QPAXRD) OF ROCK, ORE AND CONCENTRATES. By A.A.Brovkin, Sci.-Ind.Union "GRANT", Geological Committee, Russia.

In early eighties was developed and widely introduced in the geological service of the FSU unification system (QPAXRD). Later on this system was always improved to fit computing technology progress. QPAXRD system is based on: 1) inner standard method, i.e.  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> powder certified according to the intensity ratio of diffraction reflections; 2) grinding unification, trial and standard homogenization, texture factor consideration; 3) diffraction spectra survey (DS) in the discrete scanning regime; 4) evaluation of the analysis results by the intermethodical control data and intralaboratory 20% reproducibility control. Within the framework of the unification system there are widely approved in practice Chung calibration coefficients (1974) for over 100 minerals. In one test up to 10-15 minerals content is determined. Peaks superposition factor was taken via the strip-tease method for DS stage removal of DS discrete minerals whose spectra were earlier recorded in DS processing program. Under one-stage samples surveying (2 sec. exposition in the dispersion scanning step ( $\delta$ ) of the analysis results in the content interval of 5-10%, 10-30%, and 30-50% was equal to 12%, 8% and 6%, respectively). At two-stage surveying  $\delta$  reduces by 2-3 times. However, a total time of DS surveying increases by 1.5 time.

**PS-08.01.39**

THE CRYSTAL STRUCTURE CLASSIFICATION ON CATION TYPE NETS FOR THE FLUORIDES WITH HEAVY METALS.

By S. V. Borisov\*, N. A. Bliznyuk, N. V. Podberezhskaya, Institute of Inorganic Chemistry of Siberian Department of Russian Academy of Sciences, Novosibirsk, Russia.

Complex fluorides including those of Zr, U, Th La-Lu have been analysed crystallographically proceeding from the assumption that a main factor determining crystal structures of compounds with heavy atoms is a mutual arrangement of these atoms. The crystal chemistry analysis involved: 1) determination of close packed crystallographic layers (filled with cations); 2) construction of the cation nets in the layers; 3) formulation of the rules